Stepan Stepanovic

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Density functional approximations for consistent spin and oxidation states of oxoiron complexes. International Journal of Quantum Chemistry, 2020, 120, e26121.	2.0	10
2	Improvement of d–d interactions in density functional tight binding for transition metal ions with a ligand field model: assessment of a DFTB3+ <i>U</i> model on nickel coordination compounds. Physical Chemistry Chemical Physics, 2020, 22, 27084-27095.	2.8	3
3	Lewis versus BrÃ,nsted Acid Activation of a Mn(IV) Catalyst for Alkene Oxidation. Inorganic Chemistry, 2019, 58, 14924-14930.	4.0	20
4	The Irony of Manganocene: An Interplay between the Jahn–Teller Effect and Close-Lying Electronic and Spin States. Journal of Chemical Information and Modeling, 2019, 59, 1806-1810.	5.4	4
5	A Nonâ€Heme Iron Photocatalyst for Lightâ€Driven Aerobic Oxidation of Methanol. Angewandte Chemie, 2018, 130, 3261-3265.	2.0	5
6	A Nonâ€Heme Iron Photocatalyst for Lightâ€Driven Aerobic Oxidation of Methanol. Angewandte Chemie - International Edition, 2018, 57, 3207-3211.	13.8	34
7	Selective Photo-Induced Oxidation with O ₂ of a Non-Heme Iron(III) Complex to a Bis(imine-pyridyl)iron(II) Complex. Inorganic Chemistry, 2018, 57, 4510-4515.	4.0	5
8	Structural diversity of isothiocyanato Cd(II) and Zn(II) Girard's T hydrazone complexes in solution and solid state: effect of H-bonding on coordination number and supramolecular assembly of Cd(II) complex in solid state. Structural Chemistry, 2018, 29, 1797-1806.	2.0	10
9	The role of spin states in the catalytic mechanism of the intra- and extradiol cleavage of catechols by O ₂ . Organic and Biomolecular Chemistry, 2017, 15, 7860-7868.	2.8	9
10	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. Journal of Computational Chemistry, 2017, 38, 2171-2185.	3.3	39
11	Unique mononuclear Mn ^{II} complexes of an end-off compartmental Schiff base ligand: experimental and theoretical studies on their bio-relevant catalytic promiscuity. Dalton Transactions, 2016, 45, 12409-12422.	3.3	55
12	Resolving the origin of the multimode Jahn–Teller effect in metallophthalocyanines. Physical Chemistry Chemical Physics, 2016, 18, 29122-29130.	2.8	10
13	Decarbonylative Dibromination of 5-Phenylthiophene-2-carbaldehyde with Bromine. Synthesis, 2016, 48, 4423-4430.	2.3	3
14	High-yielding method for preparation of carbocyclic or <i>N</i> -containing heterocyclic β-keto esters using <i>in situ</i> activated sodium hydride in dimethyl sulphoxide. Green Chemistry Letters and Reviews, 2016, 9, 61-68.	4.7	3
15	Challenges in assignment of orbital populations in a high spin manganese(<scp>iii</scp>) complex. Dalton Transactions, 2016, 45, 6702-6708.	3.3	11
16	Magnetic Anisotropy in "Scorpionate―Firstâ€Row Transitionâ€Metal Complexes: A Theoretical Investigation. Chemistry - A European Journal, 2015, 21, 3716-3726.	3.3	12
17	Experimental and theoretical investigation of octahedral and square-planar isothiocyanato complexes of Ni(II) with acylhydrazones of 2-(diphenylphosphino)benzaldehyde. Polyhedron, 2015, 89, 271-279.	2.2	13
18	Spin state relaxation of iron complexes: The case for OPBE and S12g. Journal of the Serbian Chemical Society, 2015, 80, 1399-1410.	0.8	15

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19	A density functional study of the spin state energetics of polypyrazolylborato complexes of first-row transition metals. Physical Chemistry Chemical Physics, 2014, 16, 14514.	2.8	20
20	Role of Spin State and Ligand Charge in Coordination Patterns in Complexes of 2,6-Diacetylpyridinebis(semioxamazide) with 3d-Block Metal Ions: A Density Functional Theory Study. Inorganic Chemistry, 2013, 52, 13415-13423.	4.0	19